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Division of Environmental Chemistry - Solution and Interface Chemistry -

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Bioinformatique Structurale Institut Pasteur, France, 12 January 2005

University of Pittsburgh School of Medicine, USA, 28 February 2005

University of Pennsylvania, USA, 14 April 2005

The Pennsylvania State University, USA, 11 October 2005

University of Michigan, USA, 7 - 19 November 2005

Scope of Research

Structure and dynamics of a variety of ionic and nonionic solutions of physical, chemical, and biological interests are systematically studied by NMR and computer simulations from ambient to extreme conditions. High pressures and high temperatures are employed to shed light on microscopic controlling factors for the structure and dynamics of solutions. Static and dynamic NMR of endocrine disruptors, anesthetics, peptides, and proteins in model and cell membranes are also investigated.

Research Activities (Year 2005)

Presentations

Mobility and Location of Anesthetics in Lipid Bilayer Membranes by High-Resolution, High-Field-Gradient NMR, Okamura E, Nakahara M, The 7th International Conference on Mechanisms of Anesthesia, 25 - 27 February.

Molecular Dynamics Simulation of Solubilization by Micelle, Liang Kuo-Kan, Matubayasi N, Nakahara M, The 85th Annual Meeting of the Chemical Society of Japan, 26 - 29 March, and 3 related presentations in other symposia.

Limited Slowdown of Molecular Diffusion in Confined Fluid Lipid Membranes, Okamura E, Wakai C, Matubayasi N, Nakahara M, The 72nd Meeting of the Electrochemical Society of Japan, 1 - 3 April (Invited), and 6 related presentations in other meetings and symposia.

Method of Energy Representation as an Approach to the Solvation Free Energy, Matubayasi N, EMLG/JMLG Annual Meeting 2005 (Invited), 4 - 8 September, and 5 related presentations in other meeting, symposium, and conference.

Self-Diffusion of Light and Heavy Water in Sub- and Supercritical Conditions Studied by a New High-Temperature Multinuclear Diffusion NMR Probe, Yoshida K, Wakai C, Matubayasi N, Nakahara M, The General Symposium of Molecular Structure, 27 - 30 September, and 3 related presentations in other meetings and symposium.

Multinuclear NMR Study on Rotational Dynamics for Imidazolium-based Ionic Liquids, Wakai C, Matubayasi N, Nakahara M, 28th Symposium on Solution Chemistry of Japan, 17 - 19 November.

A New Hydrothermal C1 Chemistry: C-C Bond Formation and Disproportionations of Formaldehyde and Formic Acid, Morooka S, Wakai C, Matubayasi N, Nakahara M, Pacificchem 2005, 15 - 20 December, and 6 related presentations in other meetings and symposia.

Grants

Nakahara M, Development of Multinuclear, High-Temperature, and Diffusion Measurable NMR Probe and

A New High-Temperature Multinuclear-Magnetic-Resonance Probe and the Self-Diffusion of Light and Heavy Water in Sub- and Supercritical Conditions

A high-resolution nuclear magnetic resonance (NMR) probe (500 MHz for ^1H , Figure 1) has been developed for multinuclear pulsed field gradient spin-echo (PGSE) diffusion measurements at high temperatures up to 400 °C. The high precision is achieved by the homogeneous temperature distributions dramatically improved. The self-diffusion coefficients D for light ($^1\text{H}_2\text{O}$) and heavy ($^2\text{H}_2\text{O}$) water are distinguishably measured at subcritical temperatures of 30–350 °C on the liquid-vapor coexisting curve and at a supercritical temperature of 400 °C as a function of water density between 0.071 and 0.251 g/cm³. The D value obtained for $^1\text{H}_2\text{O}$ is 10–20% smaller than those previously reported because of the absence of the convection effect. At 400 °C, the D value for $^1\text{H}_2\text{O}$ is increased by a factor of 3.7 as the water density is reduced from 0.251 to 0.071 g/cm³. The isotope ratio $D(^1\text{H}_2\text{O})/D(^2\text{H}_2\text{O})$ decreases from 1.23 to ~1.0 as the temperature increases from 30 to 400 °C.

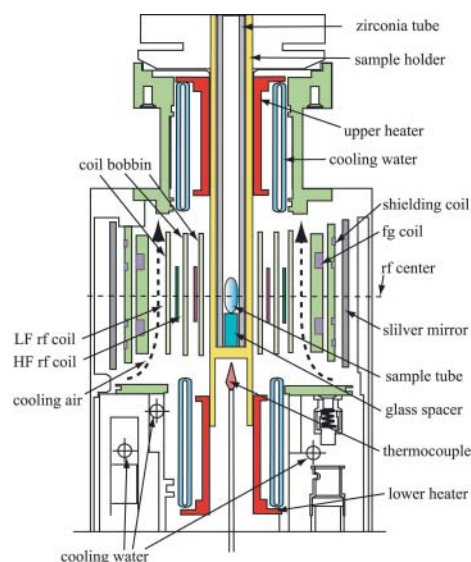


Figure 1. The cross-section view of the high-temperature multinuclear diffusion NMR probe.

Molecular Analysis of Dynamics of Supercritical Aqueous Solutions, Grant-in-Aid for Scientific Research (A), 1 April 2003 - 31 March 2006.

Nakahara M, Free-Energy Analysis of Nanoscale Aggregates of Molecules in the Method of Energy Representation, National Research Grid Initiative Project, 1 April 2003 - 31 March 2008.

Matubayasi N, Molecular Theory of the Solvation Effect on the Structural Formation and Fluctuation of Bio-

Hydrothermal Carbon-Carbon Bond Formation and Disproportionations of C1 Aldehydes: Formaldehyde and Formic Acid

Hydrothermal reaction pathways and kinetics of C1 (carbon-one) aldehydes, formaldehyde (HCHO) and formic acid ($\text{HCOOH} = \text{HOCHO}$), are studied at 225 °C without and with hydrochloric acid (HCl) up to 0.6 M (mol dm⁻³). Reactions unveiled are: (i) the self-disproportionation forming methanol and formic acid, a redox reaction between two formaldehydes, (ii) the cross-disproportionation forming methanol and carbonic acid, a redox reaction between formaldehyde and formic acid, and (iii) the acid-catalyzed C-C bond formation producing glycolic acid (HOCH_2COOH) as a precursor of the simplest amino acid, glycine (Figure 2). The reaction (iii) is a hydrothermally induced chemical evolution step from C1 aldehydes, formaldehyde and formic acid. The disproportionations (i) and (ii) are found to proceed even without base catalysts unlike the classical Cannizzaro reaction. The yield of ~90% for the glycolic acid formation and that of ~80% for the methanol formation are experimentally achieved, respectively, as a result of path weight control based on the kinetic analysis.

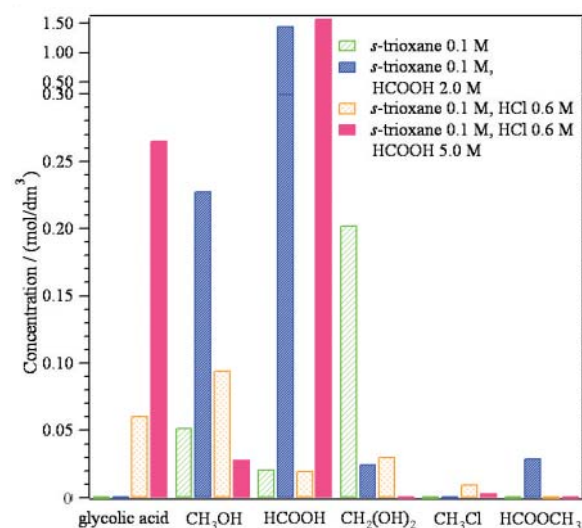


Figure 2. The product concentrations in various reaction conditions. The ordinate scale is changed at 0.30 mol/dm³.

molecules and their Aggregates, Grant-in-Aid for Scientific Research on Priority Areas, 1 April 2003 - 31 March 2008.

Matubayasi N, Toward a New Research Network between Physics and Chemistry, Grant-in-Aid for Creative Scientific Research, 1 April 2004 - 31 March 2006.

Okamura E, Molecular Dynamics in Lipid Rafts by High-Sensitivity, High-Resolution NMR, Grant-in-Aid for Scientific Research (C), 1 April 2005 - 31 March 2007.